

# Stability analysis of toxic substances within aquatic ecosystems and their effect on aquatic populations

Norman L. Miller

Environmental Research Division, Argonne National Laboratory, Argonne, IL 60439, USA

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## ABSTRACT

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A stability analysis is presented for toxic substances introduced to aquatic ecosystems and their intercompartmental relationships to aquatic populations. A specific toxin, vinyl chloride, was used in this study because an aquatic ecosystem model that includes vinyl chloride is available. The system and compartmental stability are dependent on the magnitudes and rates of transfer of vinyl chloride into, out of, and within each compartment. An 11 compartment model is presented and set up for the system eigenvalues. Compartments whose eigenvalues equal zero are the least stable because they accumulate vinyl chloride. Intercompartmental transports of vinyl chloride into and out of the filter-feeding fish compartment is incorporated into a logistic population model. This model is analyzed for growth stability as a function of vinyl chloride in the aquatic system. It is found that the population collapses when the vinyl chloride decay rate terms are greater than the growth rate term. These techniques apply to the analysis of any aquatic population where a toxic substance is present.

## INTRODUCTION

Anthropogenically produced toxic substances that enter the aquatic food chain represent a serious health threat to humans and to the inhabitants of such polluted ecosystems. The ability of an aquatic ecosystem to restore itself to the pre-pollution state is directly related to the compartmental retention times and exchange rates among compartments and the transport

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Correspondence to: N.L. Miller, Environmental Research Division, Argonne National Laboratory, Argonne, IL 60439, USA.

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rates out of the system. The effect of a toxic substance can be best understood by measuring its presence throughout an aquatic system and by determining the rates of its transport between and storage within compartments (Hutchinson, 1957; Tsivoglou, 1967; Russell-Hunter, 1970). An understanding of the compartmental and total system stability of a toxic substance can be achieved with the use of conceptual models.

This study addresses stability and compartmental responses for the well-studied toxic pollutant vinyl chloride. The techniques used are applicable to virtually any toxic substance and aquatic ecosystem, if the system, compartmental rates, and the toxic properties are defined. This study will show compartmental and system stability and also the effect of vinyl chloride (VC) on a filter-feeding fish population as a function of VC concentrations within the interdependent compartments.

#### VINYL CHLORIDE IN AQUATIC ECOSYSTEMS

Vinyl chloride is a colorless, highly flammable gas that is used in the production of polyvinyl chloride, a component of some synthetics rubbers and plastics. Production of these synthetics results in the input of VC into aquatic systems as part of industrial liquid waste (Hill et al., 1976).

Gillett et al. (1974) presented an initial model of VCs in an aquatic environment that includes VC in the water column, particulates, sediments, and the atmosphere. They also incorporated direct and indirect photochemical reactions; hydrolytic, free radical, and elimination reactions; microbial degradation; and VC in the food web. This compartmental framework is the foundation for the VC model studies of Hill et al. (1976). In these studies, compartmental pathways are constructed, and 'BEST' and 'WORST' case estimates are provided. The 'BEST' estimate approximation as defined by Hill et al. (1976) uses the most reasonable estimates of the rates for all processes as determined from laboratory results. These results indicate that all processes except volatilization are near zero. A revised version of this model is used in this study; here a nonzero atmospheric output other than the water compartment has been included (Fig. 1). In the 'WORST' case estimate, all chemical and biological transformation processes are assumed to be at rates below the level of measurement in the experimental procedure used in their determination. The revised version used in this study again includes a nonzero atmospheric output (Fig. 2).

#### STABILITY ANALYSIS

In this study, stability analysis began with a 'BEST' estimate model and then uses a 'WORST' estimate model of VC in the aquatic environment

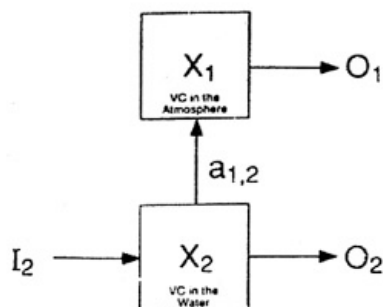


Fig. 1. 'BEST' estimate model.  $X_1$ , atmosphere compartment;  $X_2$ , water compartment;  $I_2$ , VC input to  $X_2$ ;  $O_1$ , VC output from  $X_1$ ;  $O_2$ , VC output from  $X_2$ .

(Hill et al., 1976). Figure 1 illustrates the simple, two-compartment model (water and atmosphere). The input ( $I_2$ ) and the outputs ( $O_1$ ,  $O_2$ ) are described here as constants operating in the atmospheric (1) and water (2) compartments. The net transport of VC between the water and atmosphere ( $a_{1,2}$ ) is one-directional because of the volatility of VC (Gillett et al., 1974). Atmospheric deposition processes are neglected. This two-compartment system is represented mathematically as follows:

$$dX_1/dt = a_{1,2}X_2 - O_1X_1 \quad (1a)$$

$$dX_2/dt = I_2 - (O_2 + a_{1,2})X_2 \quad (1b)$$

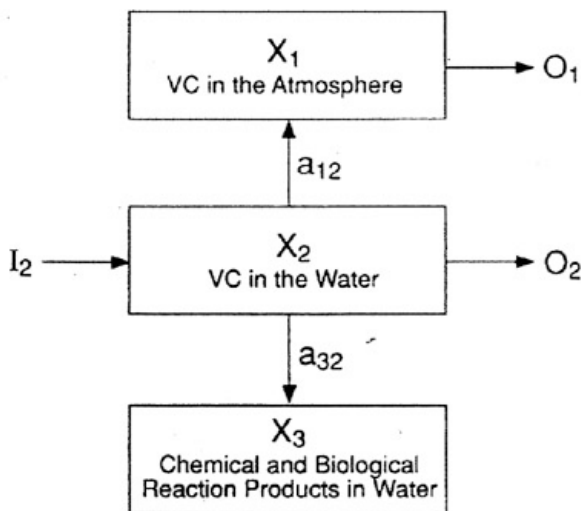


Fig. 2. 'WORST' estimate model.  $X_1$ , VC in atmosphere;  $X_2$ , VC in water;  $X_3$ , VC in chemical and biological reaction products in water;  $I_2$ , VC input to  $X_2$ ;  $O_2$ , VC output from  $X_2$ ;  $O_1$ , VC output from  $X_1$ ;  $O_3$ , VC output from  $X_3$ .

The solution of these equations is:

$$X_1(t) = X_1^* + (X_1(0) - X_1^*) \exp(-O_1 t) \quad (2a)$$

$$X_2(t) = X_2^* + (X_2(0) - X_2^*) \exp[-(O_2 + a_{1,2})t] \quad (2b)$$

where  $X_2^* = I_2/(O_2 + a_{1,2})$  and  $X_1^* = X_2^* a_{1,2}/O_1$ . Here  $X_1^*$  and  $X_2^*$  represent the steady-state equilibrium values for compartments (1) and (2). An equilibrium-centered perturbation analysis will remove the assumed constant values  $I_2$  from equation (1b). Let  $X_i = X_i^* + x_i$ , where  $x_i/X_i^* \ll 1$  for  $i = 1, 2$ , and  $X_i^*$  are the constant equilibrium values. Now  $dX_i/dt = dx_i/dt$ , and:

$$dx_1/dt = a_{1,2}x_2 - O_1x_1 \quad (3a)$$

$$dx_2/dt = -(O_2 + a_{1,2})x_2 \quad (3b)$$

The community matrix for this system is defined as:

$$\tilde{A} = \begin{vmatrix} -O_1 & a_{1,2} \\ 0 & -(O_2 + a_{1,2}) \end{vmatrix} = \begin{vmatrix} -\lambda_1 & a_{1,2} \\ 0 & -\lambda_2 \end{vmatrix} \quad (4)$$

where the system eigenvalues are defined as  $\lambda_1 = O_1$ , and  $\lambda_2 = (O_2 + a_{1,2})$ . The solution to  $dx_i/dt = \tilde{A}x_i$  has the general form  $x_i(t) = C_0 \exp(-C_1 t)$ , where  $C_0$  and  $C_1$  are constants. This solution implies that all of the perturbations within this system have the same time dependence. In matrix form this is expressed as  $\tilde{A}x = \lambda x$  or  $(\tilde{A} - \lambda \tilde{I}) = 0$ , where  $\tilde{I}$  is the identity matrix. The trivial solution is  $x = 0$ , but the nontrivial solution occurs when the determinant is equal to zero:

$$|\tilde{A} - \lambda \tilde{I}| = \begin{vmatrix} -(\lambda + \lambda_1) & a_{1,2} \\ 0 & -(\lambda + \lambda_2) \end{vmatrix} = (\lambda + \lambda_1)(\lambda + \lambda_2) = 0 \quad (5)$$

This is the secular equation; it gives the eigenvalues of this system. The equilibrium points are at  $\lambda = \lambda_1, \lambda_2$ , which both are real and positive. Substituting the eigenvalues back into equations (2a, b) indicates that  $X_2$  has a stable component with respect to VC perturbations. A VC perturbation in  $X_2$  is illustrated in Fig. 3 as an abrupt increase in the VC concentration in  $X_2$ , which exponentially decays back to an equilibrium value. The rate in which a perturbed compartment returns to a stable equilibrium depends on the compartment size and the magnitudes of VC transport into and out of the perturbed compartment. If  $X_1 \gg X_2$ , then a neutral situation results. In this case the transport of VC from the water compartment into the atmosphere is very small compared to the atmosphere compartment. However, if conditions represented, a mountainous valley where an atmospheric inversion is often present ( $O_1$  is very small),

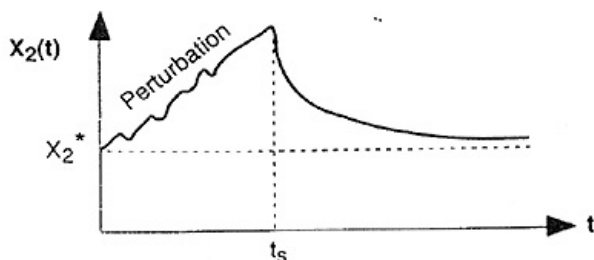


Fig. 3. Water compartment is perturbed by  $\Delta t$  input of VC. Over time this disturbance reaches and equilibrium.

then significant effects to  $X_1$  would be likely. This last case would imply global stability with a tendency toward local instability in some external conditions.

The 'WORST' estimate case is defined here as a three-compartment system where chemical and biological reaction products in water are the third compartment (Fig. 2). This model and the 'BEST estimate' model will give the extreme ranges of possible outcomes. The three-component system is represented mathematically as follows:

$$dX_1/dt = a_{1,2}X_2 - O_1X_1 \quad (6a)$$

$$dX_2/dt = I_2 - (O_2 + a_{1,2} + a_{3,2})X_2 \quad (6b)$$

$$dX_3/dt = a_{3,2}X_2 - O_3X_3 \quad (6c)$$

where  $\lambda_1 = O_1$ ,  $\lambda_2 = O_2 + a_{1,2} + a_{3,2}$ ,  $\lambda_3 = O_3$ . The solutions to equations (6a, b, c) are:

$$X_1(t) = X_1^* + [X_1(0) - X_1^*] \exp(-\lambda_1 t) \quad (7a)$$

$$X_2(t) = X_2^* + [X_2(0) - X_2^*] \exp(-\lambda_2 t) \quad (7b)$$

$$X_3(t) = X_3^* + [X_3(0) - X_3^*] \exp(-\lambda_3 t) \quad (7c)$$

where  $X_2^* = I_2/\lambda_2$ ,  $X_1^* = X_2^*a_{1,2}/\lambda_1$  and  $X_3^* = X_2^*a_{3,2}/\lambda_3$ .

Equilibrium-centered perturbation analysis has a form similar to equations (3a, b):

$$dx_1/dt = a_{1,2}x_2 - \lambda_1x_1 \quad (8a)$$

$$dx_2/dt = -\lambda_2x_2 \quad (8b)$$

$$dx_3/dt = a_{3,2}x_2 - \lambda_3x_3 \quad (8c)$$

with a community matrix defined as

$$\tilde{A} = \begin{vmatrix} -\lambda_1 & a_{1,2} & 0 \\ 0 & -\lambda_2 & 0 \\ 0 & a_{3,2} & -\lambda_3 \end{vmatrix} \quad (9)$$

$$= -(\lambda + \lambda_1)(\lambda + \lambda_2)(\lambda + \lambda_3) = 0 \quad (10)$$

where  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_3$  are positive and real. Substituting the eigenvalues back into equations (7a, b, c) again indicates that there is stability at  $\lambda = -\lambda_1$ ,  $-\lambda_2$ , and  $-\lambda_3$ .

The sensitivities of each compartment equilibrium value to changes in the input, output, and transfer rates are critical in evaluating a system response. In this system,  $X_1^* = a_{1,2}X_2^*/\lambda_1$ ,  $X_2^* = I_2/\lambda_2$ , and  $X_3^* = a_{3,2}X_2^*/\lambda_3$ . These values are subject to a sensitivity analysis in  $O_1$ ,  $I_2$ ,  $O_2$ ,  $O_3$ ,  $a_{1,2}$ , and  $a_{3,2}$ . Each equilibrium value  $x_i^*$  is expressed here as a linear function of input, outputs, and transfer rates which are given as perturbations about a mean constant value. That is,  $O_1 = O_1^0(1 + P_{O_1})$ ,  $O_3 = O_3^0(1 + P_{O_3})$ ,  $I_2 = I_2^0(1 + P_{I_2})$ ,  $a_{1,2} = a_{1,2}^0(1 + P_{a_{1,2}})$ , and  $a_{3,2} = a_{3,2}^0(1 + P_{a_{3,2}})$ . Here  $O_1^0$ ,  $I_2^0$ ,  $O_2^0$ ,  $O_3^0$ ,  $a_{1,2}^0$ , and  $a_{3,2}^0$  are mean constant values, while  $P_{O_1}$ ,  $P_{O_2}$ ,  $P_{O_3}$ ,  $P_{I_2}$ ,  $P_{a_{1,2}}$ , and  $P_{a_{3,2}}$  are fractional changes. Linear approximations for each equilibrium value is expressed as:

$$X_1^*(O_1, O_2, I_2, a_{1,2}, a_{3,2}) = X_1^*(O_1) + X_1^*(O_2) + X_1^*(I_2) + X_1^*(a_{1,2}) + X_1^*(a_{3,2}) \quad (11a)$$

$$X_2^*(O_2, I_2, a_{1,2}, a_{3,2}) = X_2^*(O_2) + X_2^*(I_2) + X_2^*(a_{1,2}) + X_2^*(a_{3,2}) \quad (11b)$$

$$X_3^*(O_2, I_2, O_3, a_{1,2}, a_{3,2}) = X_3^*(O_2) + X_3^*(I_2) + X_3^*(O_3) + X_3^*(a_{1,2}) + X_3^*(a_{3,2}) \quad (11c)$$

The sensitivity analysis to  $X_1^*(O_1)$  is given below. Sensitivities to all of the remaining terms in equations (11 a, b, c) are given in Table 1.

$$\begin{aligned} & [X_1^*(O_1) - X_1^*(O_1^0)]/X_1^*(O_1^0) \\ &= \frac{(a_{1,2}^0 I_2^0)/[O_1(O_2^0 + a_{1,2}^0 + a_{3,2}^0)] - (a_{1,2}^0 I_2^0)/[O_1^0(O_2^0 + a_{1,2}^0 + a_{3,2}^0)]}{(a_{1,2}^0 I_2^0)/[O_1^0(O_2^0 + a_{1,2}^0 + a_{3,2}^0)]} \\ &= (O_1^0 - O_1)/O_1 = -P_{O_1}/(1 + P_{O_1}) \end{aligned} \quad (12)$$

and

$$X_1^*(O_1) = X_1^*(O_1^0)[1 - P_{O_1}/(P_{O_1} + 1)] = X_1^*(O_1^*)[1 + S_{O_1}] \quad (13)$$

TABLE 1

Sensitivity analysis of terms in equations (11a, b, c) \*

$S_j$	$X_1^*(j)$	$X_2^*(j)$	$X_3^*(j)$
$S_{O_1}$	$-P_{O_1}/(P_{O_1}+1)$	-	-
$S_{O_2}$	$-P_{O_2}/(P_{O_2}+1+C_{O_2})$	$-P_{O_2}/(P_{O_2}+1+C_{O_2})$	$-P_{O_2}/(P_{O_2}+1+C_{O_2})$
$S_{O_3}$	-	-	$-P_{O_3}/(P_{O_3}+1)$
$S_{I_2}$	$P_{I_2}$	$P_{I_2}$	$P_{I_2}$
$S_{a_{1,2}}$	$\frac{P_{a_{1,2}}(a_{3,2}^0 + O_2^0)}{P_{a_{1,2}} + 1 + C_{a_{1,2}}}$	$\frac{-P_{a_{1,2}}}{P_{a_{1,2}} + 1 + C_{a_{1,2}}}$	$\frac{-P_{a_{1,2}}}{P_{a_{1,2}} + 1 + C_{a_{1,2}}}$
$S_{a_{3,2}}$	$\frac{-P_{a_{3,2}}}{P_{a_{3,2}} + 1 + C_{a_{3,2}}}$	$\frac{-P_{a_{3,2}}}{P_{a_{3,2}} + 1 + C_{a_{3,2}}}$	$\frac{P_{a_{3,2}}(a_{1,2}^0 + O_2^0)}{P_{a_{3,2}} + 1 + C_{a_{3,2}}}$

$$* C_{O_2} = (a_{1,2}^0 + a_{3,2}^0)/O_2^0 \quad C_{O_3} = (a_{1,2}^0 + a_{3,2}^0)$$

$$C_{a_{1,2}} = (O_2^0 + a_{3,2}^0)/a_{1,2}^0 \quad C_{a_{3,2}} = O_2^0 + a_{1,2}^0/a_{3,2}^0$$

The general form for the sensitivity of the system of equations is::

$$X_i^* = X_1^*(O_1^0)(1 + S_{O_1}) + X_i^*(O_2^0)(1 + S_{O_2}) + X_i^*(I_2^0)(1 + S_{I_2})$$

$$+ X_i^*(a_{1,2}^0)(1 + S_{a_{1,2}}) + X_i^*(a_{3,2}^0)(1 + S_{a_{3,2}}) \quad (14)$$

Positive changes in  $I_2$  linearly increase each compartment as expected. Increases in output  $O_2$  indicate equal but small decreases for each compartment that depend on the magnitude of  $C_{O_2}$ . The most sensitive parameters are  $a_{1,2}$  and  $a_{3,2}$  depending on which compartment is being evaluated. The sensitivity of  $a_{1,2}$  is similar to that of  $O_2$  for  $X_2^*$  and  $X_3^*$ , but now there is a dependence on the magnitude of  $C_{a_{3,2}}$ . Similarly for  $a_{3,2}$ ,  $X_1^*$  and  $X_2^*$  show the same dependence as  $C_{a_{3,2}}$ . However,  $X_1^*$  is very sensitive to changes in  $a_{1,2}$ , as  $X_3^*$  is to  $a_{3,2}$ , as is illustrated in Table 1. Variations in  $O_1$  and  $O_3$  affect only their respective compartmental equilibria,  $X_1^*$  and  $X_3^*$ . System perturbations and compartmental responses will behave according to the above linear sensitivity analysis. The most important aspects of this type of study are the magnitudes of each parameter and their interdependencies. Each parameter determines the values of the equilibrium concentrations in proportion to these results.

The 'BEST' estimate and 'WORST' estimate models indicate only trends in system stability as a function of the VC magnitudes and rates and of the compartments' abilities to reach equilibrium. Clearly a full-system model is necessary to understand the local stability of each compartment and the global stability of the entire system. Hill et al. (1976) provided a system diagram for their model of VC in an aquatic system (Fig. 4). This

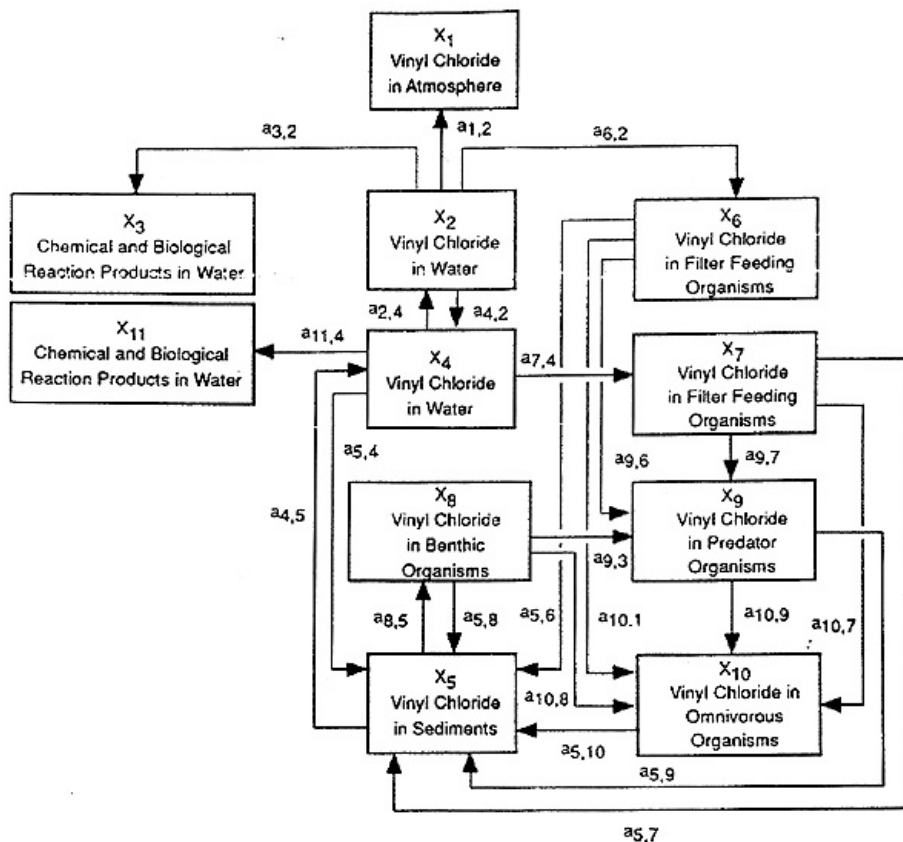


Fig. 4. System model of VC in a stratified lake with a simple, idealized flood web.

TABLE 2

Set of equations describing the 11-compartment aquatic ecosystems

Compartment	Linear equation	Eigenvalue ( $\lambda_i$ )
1	$dX_1/dt = a_{1,2}X_2$	$\lambda_1 = 0$
2	$dX_2/dt = a_{2,4}X_4 - \lambda_2X_2$	$\lambda_2 = a_{1,2} = a_{3,2} + a_{4,2} + a_{6,2}$
3	$dX_3/dt = a_{3,2}X_2$	$\lambda_3 = 0$
4	$dX_4/dt = a_{4,2}X_2 + a_{4,5}X_5 - \lambda_4X_4$	$\lambda_4 = a_{2,4} + a_{5,4} + a_{7,4} + a_{11,4}$
5	$dX_5/dt = a_{5,4}X_4 + a_{5,6}X_6 + a_{5,7}X_7 + a_{5,8}X_8 + a_{5,9}X_9 + a_{5,10}X_{10} - \lambda_5X_5$	$\lambda_5 = a_{4,5} + a_{8,5}$
6	$dX_6/dt = a_{6,2}X_2 - a_6X_6$	$\lambda_6 = a_{5,6} + a_{9,6} + a_{10,6}$
7	$dX_7/dt = a_{7,4}X_4 - a_7X_7$	$\lambda_7 = a_{5,7} + a_{9,7} + a_{10,7}$
8	$dX_8/dt = a_{8,5}X_5 - a_8X_8$	$\lambda_8 = a_{5,8} + a_{9,2}$
9	$dX_9/dt = a_{9,6}X_6 + a_{9,7}X_7 + a_{9,8}X_8 - \lambda_9X_9$	$\lambda_9 = a_{5,9} + a_{10,9}$
10	$dX_{10}/dt = a_{10,6}X_6 + a_{10,7}X_7 + a_{10,9}X_9 - \lambda_{10}X_{10}$	$\lambda_{10} = a_{5,10}$
11	$dX_{11}/dt = a_{11,4}X_4$	$\lambda_{11} = 0$



simple model represents VC in an idealized food web and omits several feedbacks (atmospheric deposition, resuspension, plankton, fecal, etc.). As in equations (1a, b) and (6a, b, c), a set of linear equations and eigenvalues is defined in Table 2.

More detailed systems of equations can be built up with the present technique and handled in the same fashion as above. Equations in Table 2 whose eigenvalues are equal to zero designate VC sinks. It is assumed (Fig. 4) that this is a closed lake system, that there are no significant outlets for  $O_1$ ,  $O_2$ , and  $O_3$ . The community matrix for this system is defined as:

$$\bar{A} = \begin{matrix} & 0 & a_{1,2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & 0 & -\lambda_2 & 0 & a_{2,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & 0 & a_{3,2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & 0 & a_{4,2} & 0 & -\lambda_4 & a_{4,5} & 0 & 0 & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & a_{5,4} & -\lambda_5 & a_{5,6} & a_{5,7} & a_{5,8} & a_{5,4} & a_{5,10} & 0 \\ & 0 & a_{6,2} & 0 & 0 & 0 & -\lambda_6 & 0 & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & a_{7,4} & 0 & 0 & -\lambda_7 & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & 0 & a_{8,5} & 0 & 0 & -\lambda_8 & 0 & 0 & 0 \\ & 0 & 0 & 0 & 0 & 0 & a_{9,6} & a_{9,7} & a_{9,8} & -\lambda_9 & 0 & 0 \\ & 0 & 0 & 0 & 0 & 0 & a_{10,6} & a_{10,7} & a_{10,8} & a_{10,9} & -\lambda_{10} & 0 \\ & 0 & 0 & 0 & a_{11,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{matrix} \quad (15)$$

where  $\lambda_1 = \lambda_3 = \lambda_{11} = 0$ ,  $\lambda_4 = \lambda_{10}$ ,  $\lambda_5 = \lambda_9$ , and  $\lambda_6 = \lambda_8$ . The secular equation produces an 11th-degree equation in  $\lambda$  whose solution determines the eigenvalues for this system of equations. The eigenvalues correspond to those given in Table 2. Compartmental magnitudes and rates determine local stability. This system exhibits local and global stability. The ratio  $X_4/X_2$  and the ratio  $a_{2,4}/a_{4,2}$  indicate the sizes of stratified layers and the mixing between the layers. An unstable case would occur when  $X_4(t)/X_2(t) \gg 1$ . This is the situation where  $X_2(t)$  is very small compared to  $X_4(t)$  and has an input from  $X_2(t)$  ( $a_{2,4}$ ) that is much greater than the output from  $X_2(t)$  ( $\lambda_2 X_2(t)$ ). Other compartments and transfers are subject to similar instabilities; such situations can force the entire system to become unstable. VC could accumulate at a devastating rate because of small or zero eigenvalues (e.g., in fatty tissue of fish). The effect that a toxic substance has on a biological compartment within an aquatic ecosystem is detailed in the following section, which uses the model in Fig. 4 (Hill et al., 1976).

#### FISH POPULATION AS A FUNCTION OF VINYL CHLORIDE

The pathways of a toxic substance within an aquatic ecosystem depend on the rates and residences between and among compartments. Under-

standing the effect of this intercompartmental exchange of VC on the growth rate of filterfeeding fish will highlight the usefulness of this approach. This analysis will indicate the overall quantitative effect of VC has on the growth rate of filter-feeding fish and the compartments from which this toxin is most significant. Figure 4 indicates that the VC concentration in the bottom layer filter-feeding fish has one input, VC transported from the water compartment,  $a_{7,4}X_4(t)$ , and three outputs, to sediments ( $a_{5,7}$ ), predator organisms ( $a_{8,7}$ ), and omnivorous organisms ( $a_{10,7}$ ). This model can easily be expanded to include other compartments as they become important. The particular and homogeneous solution for compartment 7 in Table 2 has the form:

$$X_7(t) = X_7(0) e^{-\lambda_7 t} + X_7^* + X_4^* \quad (16)$$

The population growth rate for compartment 7,  $r(X_7, t)$ , and the carrying capacity,  $K(X_7, t)$ , can be approximated as linear functions with first-order dependence on  $X_7(t)$  as follows:

$$r(X_7, t) = r(0) - \gamma X_7(t) \quad (17a)$$

$$K(X_7, t) = K(0) - \nu X_7(t) \quad (17b)$$

Here  $r(0)$  and  $K(0)$  are the initial growth rate and the carrying capacity, and  $\gamma$  and  $\nu$  are constants. Applying a logistic population model (Volterra, 1926) gives the following:

$$\frac{dN}{dt} = r(X_7, t) N(t) \left( 1 - \frac{N(t)}{K(X_7, t)} \right) \quad (18)$$

where  $N(t)$  is the time-dependent population of filter-feeding fish. For simplicity, it is assumed here that toxin effects all age classes similarly. Defining  $\eta(t) = N(t)/K(X_7, t)$  and substituting equation (17a) for  $r(X_7, t)$  results in the following integral:

$$\int_{\eta(0)}^{\eta(t)} \frac{d\eta}{\eta(1-\eta)} = \int_0^t \{ r(0) - \gamma [X_7(0) e^{-\lambda_7 t} + X_7^* + X_4^*] \} dt \quad (19)$$

whose solution is

$$\eta(t) = \eta(0) \{ [1 - \eta(0)] \exp[-r(0)t + J(1 - e^{-\lambda_7 t}) + Ht] + \eta(0) \}^{-1} \quad (20)$$

where the constants  $J = \gamma X_7(0)/\lambda_7$  and  $H = \lambda(X_7^* + X_4^*)$ . The presence of VC in this aquatic ecosystem quantitatively affects the filter-feeding fish population as terms  $J$  and  $H$  in equation (20). Evaluation of  $J(1 - e^{-\lambda_7 t})$  and  $Ht$  reveals that if  $H > r(0)$ , then  $\eta(t)$  approaches zero as  $t$  goes to

infinity. If  $H < r(0)$ , then  $\eta(t)$  approaches unity as  $t$  goes to infinity. That is,  $\eta(t)$  approaches its carrying capacity over time only if the initial growth rate is greater than the rate effect term  $H$ . The effect of VC removal rates from compartment 7 is seen in term  $J(1 - e^{-\lambda_7 t})$ . The initial removal value of zero is not felt until time periods on the order of  $1/\lambda_7$  have passed. This initial removal value is again hinged to each rate term in  $X_7$ , which has a stabilizing effect similar to the earlier discussions for the 'BEST' and 'WORST' estimate models. After a time interval  $t \gg 1/\lambda_7$ ,  $J(1 - e^{-\lambda_7 t})$  approaches  $\gamma X_7(0)/\lambda_7$ , the steady state.

Further evaluation of the effects of VC on the growth and stability within a time-dependent population is made possible by rewriting equation (20) as:

$$\eta(t) = \frac{1}{1 + We^{-St}} \quad (21)$$

where now  $S(t) = r(0)t - J(1 - e^{-\lambda_7 t}) - Ht$  and  $W = (1 - \eta(0))/\eta(0)$ . Population stability is analyzed by letting  $\eta(t) = \eta^* + X(t)$ , where  $\eta^*$  is the equilibrium population and  $X(t)$  is the time-dependent population perturbation. Figure 5 shows that the filter-feeding fish population will equalize at  $\eta(t) = 1$  (the carrying capacity) for  $S > 0$  and at  $\eta(t) = 0$  for  $S < 0$ . Graphically this is a double sigmoid growth and decay curve with symmetry about  $\eta(0)$ . Here  $\eta(S < 0)$  and  $\eta(S > 0)$  are the growth rate extremes; they are illustrated in Fig. 5 as curves a and e respectively. Section I in Fig. 5 is the region where  $r(0)t > J(1 - e^{-\lambda_7 t}) + Ht$ ; it represents population growth. The exponent in equation (21) decays with time, and a normalized equilibrium value (carrying capacity) is approached. Curve b lies in section I, and its sigmoidal growth is dependent on the magnitude of  $r(0) - J(1 - e^{-\lambda_7 t}) + Ht$ . The population growth approaches zero as this value approaches zero. This resultant zero slope at  $\eta(t) = \eta(0)$  is a steady-state situation that is represented by curve c in Fig. 5. Curve d is the case where  $r(0)t < J(1 - e^{-\lambda_7 t}) + Ht$ . Here the exponent grows positively with time and decreases the value of  $\eta(t)$  until a zero population is reached (until local extinction occurs). The values of the curve depend on the magnitude of  $S$ . If  $\eta(0)$  is greater than unity (the carrying capacity), the model breaks down. Figure 6 shows the case where  $\eta(0) > 1$  and  $S > 0$ , the term  $W$  is negative, and inconsistencies arise. In this situation  $\eta(t)$  asymptotically approaches infinity at  $We^{St} = 1$ . That is, as  $t$  approaches  $\ln(W)/S$ ,  $\eta(t)$  goes to infinity;  $\eta(t)$  returns from negative infinity as  $t > \ln(W)/S$ . This discontinuity occurs in the region that exceeds the limits of the model. The model is thus invalid and useless for  $\eta(0) > 1$  or  $N(0) > K$ .

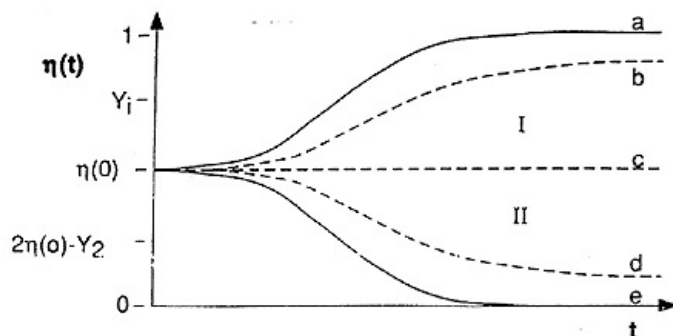


Fig. 5. Normalized filter-feeding fish growth rate as a function of VC.

Taking the derivative of equation (18) with respect to  $\eta$  illustrates the greatest and least rates of change in population:

$$\frac{d^2\eta}{dt d\eta} = S(1 - 2\eta) \quad (22)$$

Figure 7 is a plot of  $d\eta/dt$  and  $\eta$  as a function of  $S$ . The maximum (and constant) growth is at an equilibrium value  $\eta = 1/2$ . The constant decay is at  $2\eta(0) - 1/2$ . For values of  $S < 0$ ,  $d\eta/dt$  goes to zero at  $\eta = 1$ . For values of  $S < 0$ ,  $d\eta/dt$  is always negative and will reach a maximum population at  $\eta(0)$ . The constant decay at  $2\eta(0) - 1/2$  is seen as an inflection point in Fig. 5. Values of  $S > 0$  indicate that  $d\eta/dt$  goes to zero as  $\eta(t) = 0$ . This prediction is in agreement with reality; as the population

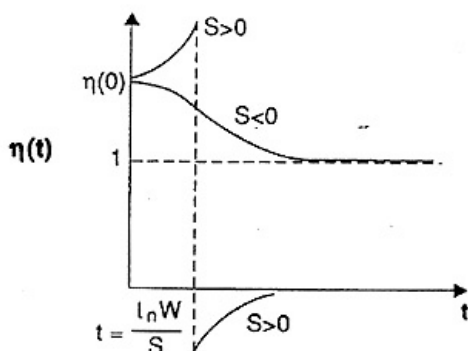


Fig. 6. Growth rate for the case where  $\eta(0) > 1$ . Model breaks down and this particular case is invalid.

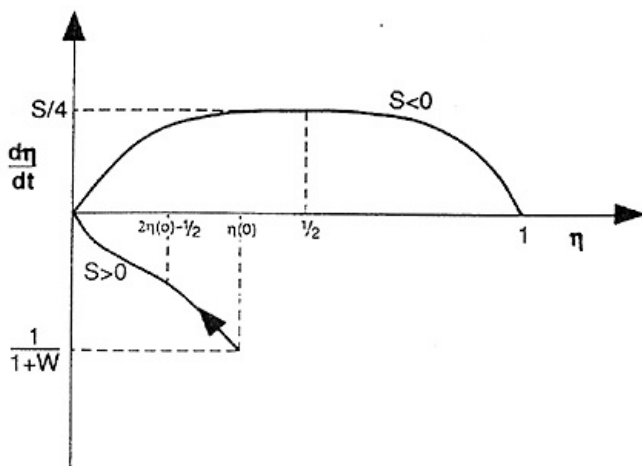


Fig. 7. Population change plotted with population as a function of  $S$ .

becomes extinct, the growth rate (decay rate) is no longer nonzero. The decay behaves as a function of  $J(1 - e^{-\lambda_1 t}) + Ht - r(0) t$ . This is an exponential linear function, and it does not reach values greater than the initial value.

## SUMMARY AND CONCLUSION

This stability analysis of toxic substances within aquatic ecosystems gave new information on compartmental and intercompartmental responses. The analysis showed that when volatilization is the significant process for toxic substance transport, the 'BEST' estimate, then the atmosphere will act as an infinite sink and there will always be stability. The length of time required for this system to return to the pre-pollution equilibrium state depends directly on the net volatilization rate. The case where chemical and biological rates are minimized, the 'WORST' estimate, is also stable and will return to its pre-pollution equilibrium state at a faster rate than the 'BEST' estimate case. This faster response is due to the inclusion of chemical and biological reactions. It was shown that the most sensitive parameters are the transfer rates between compartments. Oscillating inputs with low frequencies result in larger concentrations than high-frequency inputs throughout the entire system. A detailed system analysis for VC within the eleven-compartment model also indicates stability. This stability is initially determined at the compartment level. Some systems are less

stable than those studied here. The concentrations of toxic substances, rates, magnitudes, and retention times all vary from system to system.

The effect of a toxic substance that enters an aquatic system at some frequency and the resultant concentration of each compartment due to the transfer rates has been parameterized for a filter-feeding fish compartment. The population growth rate of filter-feeding fish is expressed as a function of the toxic substance (VC). The growth rate is quantified as a function of the transport of VC into and out of the filter-feeding fish compartment. It was shown that a range of growth rates exists and that these rates are dependent on the sign and magnitude of the term  $S$ . Effects of other variables or functions can be described within the framework of the present theory. This population analysis was set up for the general case and is applicable to any species' growth rate that is dependent on a known (or unknown) function ( $S$ ).

The implications of these results are far reaching. Aquatic ecosystems management can now quantify intercompartmental affects due to toxic substances for most any aquatic system. An understanding of compartmental stability and response will determine population trends. These tools will allow for predictive decision making.

This new approach to quantifying toxic pathways and their effects on aquatic populations gives new insight into the determination of significant transfer rates, sensitivities, compartmental interrelationships, and a host of other properties.

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#### REFERENCES

- Gillett, J.W., Hill, J., Jarvinen, A.W. and Schoor, W.P., 1974. A conceptual model for the movement of pesticides through the environment. EPA-660/2-74-024, National Environmental Research Center, Corvallis, OR, 80 pp.
- Hill, J., Kollig, H.P., Paris, D.F., Wolfe, N.L. and Zepp, R.G., 1976. Dynamic behavior of vinyl chloride in aquatic ecosystems. EPA-600/3-76-001, U.S. Environmental Protection Agency, Athens, GA, 63 pp.
- Hutchinson, G.E., 1957. A Treatise on Limnology, Vol. 1. Wiley, New York, 1015 pp.
- Russell-Hunter, G.E., 1970. Aquatic Productivity. Collier Macmillan, Toronto, Ont., 305 pp.

Tsivoglou, E.C., 1970. Tracer measurement of stream reaeration. Water Pollution Control Administration, Washington, DC, 86 pp.

Volterra, V., 1926. Variations and fluctuations of the number of individuals in animal species living together. *J. Cons. Perm. Int. Ent. Mer.*, 3: 3-51. (Reprinted in R.N. Chapman, *Animal Ecology*, New York, 1931.)